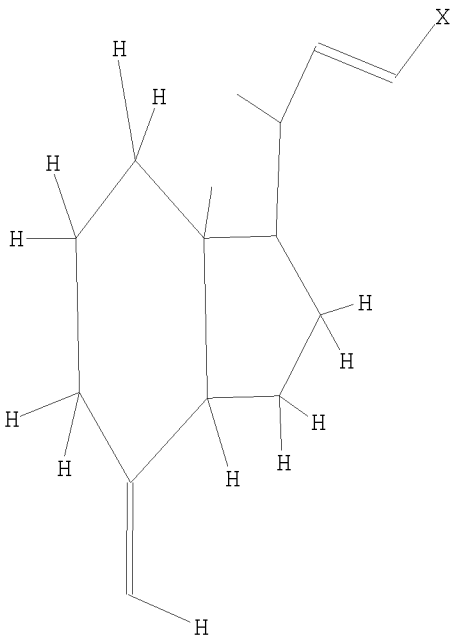
Uploading C:\Program Files\Stnexp\Queries\10579594.str

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 191.05 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 15:13:30 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 271 TO ITERATE

100.0% PROCESSED 271 ITERATIONS 16 ANSWERS
SEARCH TIME: 00.00.01

L2 16 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 191.54 191.76

FILE 'CAPLUS' ENTERED AT 15:13:44 ON 26 MAR 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 26 Mar 2010 VOL 152 ISS 14
FILE LAST UPDATED: 25 Mar 2010 (20100325/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2009

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the first quarter of 2010.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l1
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 15:13:55 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   17 TO ITERATE

100.0% PROCESSED   17 ITERATIONS   1 ANSWERS
SEARCH TIME: 00.00.01

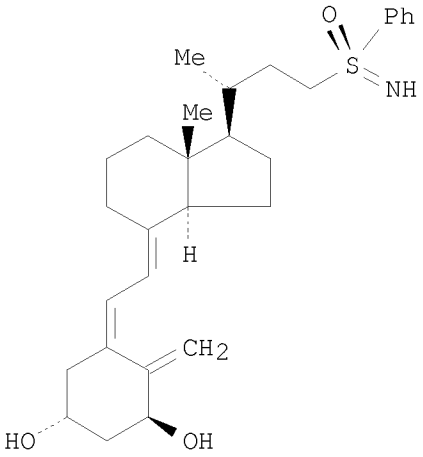
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 93 TO   587
PROJECTED ANSWERS: 1 TO   80

L3   1 SEA SSS SAM L1

L4   1 L3

=> d ibib abs hitstr
THE ESTIMATED COST FOR THIS REQUEST IS 5.81 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2004:1024083 CAPLUS
DOCUMENT NUMBER: 142:134781
TITLE: Potent, Selective and Low-Calcemic Inhibitors of CYP24 Hydroxylase: 24-Sulfoximine Analogues of the Hormone 1α,25-Dihydroxyvitamin D3
AUTHOR(S): Kahraman, Mehmet; Sinishtaj, Sandra; Dolan, Patrick M.; Kensler, Thomas W.; Peleg, Sara; Saha, Uttam; Chuang, Samuel S.; Bernstein, Galina; Korczak, Bozena; Posner, Gary H.
CORPORATE SOURCE: Department of Chemistry, School of Arts and Sciences, The Johns Hopkins University, Baltimore, MD, 21218, USA
SOURCE: Journal of Medicinal Chemistry (2004), 47(27), 6854-6863
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:134781
GI

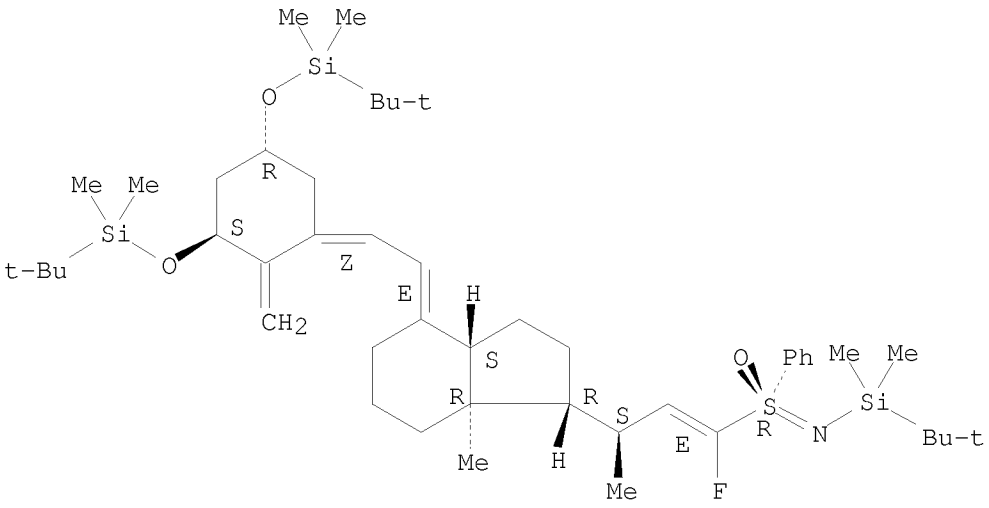


I

AB A dozen 24-sulfoximine analogs of the hormone 1α,25-dihydroxyvitamin D3 were prepared, differing not only at the stereogenic sulfoximine stereocenter but also at the A-ring. Although these sulfoximines were not active transcriptionally and were only very weakly antiproliferative, some of them are powerful hydroxylase enzyme inhibitors. Specifically, 24(S)-NH Ph sulfoximine I is an extremely potent CYP24 inhibitor (IC50 = 7.4 nM) having low calcemic activity. In addition, this compound shows high selectivity toward the CYP24 enzyme in comparison to CYP27A1 (IC50 > 1000 nM) and CYP27B (IC50 = 554 nM).
IT 825638-30-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation and CYP24 inhibitory activity of dihydroxyvitamin D3 sulfoximine analogs)
RN 825638-30-0 CAPLUS
CN Silanamine, N-[(R)-[(1E,3S)-3-[(1R,3aS,4E,7aR)-4-[(2Z)-2-[(3S,5R)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methylenecyclohexylidene]ethylidene]octahydro-7a-methyl-1H-inden-1-yl]-1-fluoro-1-buten-1-yl]oxidophenyl-λ4-sulfanylidene]-1-(1,1-dimethylethyl)-1,1-dimethyl- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



OS.CITING REF COUNT: 28 THERE ARE 28 CAPLUS RECORDS THAT CITE THIS RECORD (28 CITINGS)
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s l2
L5 7 L2

=> d 1-7 ibib abs hitstr
THE ESTIMATED COST FOR THIS REQUEST IS 40.67 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L5 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2006:1055284 CAPLUS
DOCUMENT NUMBER: 145:356983
TITLE: Procedure for the preparation of vitamin D derivatives starting with monohalovinyl compounds
INVENTOR(S): Buxade Vinas, Antonio; Conchillo Teruel, Antonio; Mola Soler, Carlos
PATENT ASSIGNEE(S): Laboratorios Vinas S.A., Spain
SOURCE: Span., 72pp.
CODEN: SPXXAD

DOCUMENT TYPE: Patent
LANGUAGE: Spanish
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ES 2234423	A1	20050616	ES 2003-2875	20031205
ES 2234423	B1	20060301		
SI 21657	A	20050630	SI 2004-326	20041202
KR 2005054857	A	20050610	KR 2004-101436	20041203

PRIORITY APPLN. INFO.: ES 2003-2875 A 20031205
OTHER SOURCE(S): CASREACT 145:356983; MARPAT 145:356983
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

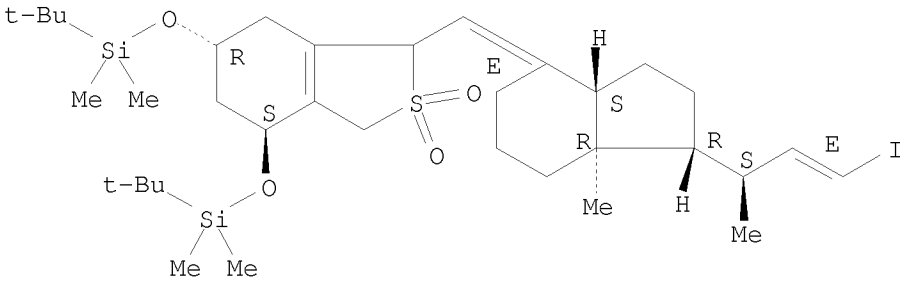
AB A procedure for the preparation of vitamin D derivs. I [A = A1, A2, A3; R1, R2, R3, R4 = H, C1-8-alkyl, C3-6-cycloalkyl, C6-14-aryl; D = H, CR5R6Y, C(:O)R5; R5, R6 = H, C1-8-alkyl, C3-6-cycloalkyl, C6-14-aryl, OR7; R7 = H, C1-8-alkyl, C3-6-cycloalkyl, C6-14-aryl; R1', R2', R3' = H, halogen, OH, protected OH, C1-6-alkyl (optionally substituted with halogen, OH, CN, NH2), C2-6-alkenyl (optionally substituted with halogen, OH, CN, NH2), C1-5-alkyl ether, di(C1-5-alkyl)amino; V = (C.tplbond.C)n; W = dienophile; Y = H, OH, protected OH; Z, Z' = H, OH, protected OH; m = 0, 1, 2; n = 0, 1; p = 0, 1, 2, 3, 4, 5, 6; whereby m + n + p ≥ 1] comprises: (a) reaction of monohalovinyl compds. II [X = halogen, selected from Cl, Br, I] with M(NR8R9) [M= alkaline metal; R8, R9 = H, C1-6-alkyl, (C1-6-alkyl)silyl, C3-6-cycloalkyl] in a solvent followed by reaction of the resulting metal vinyl compound with R5CONMeOMe or R5CHO. Alternatively the procedure can comprise: (b) reaction of monohalovinyl compds. II with MOR10 [R10 = C1-6-alkyl] in a solvent followed by reaction with R5CONMeOMe or R5CHO; (c) reaction of II with R10Li followed by reaction with 2-R5-2-R6-oxirane; (d) reaction of II with (T)oM'(CR4R4)pCHR6R6 [M' = Li, Mg, Zn, Al, Zr, B, Sn; T = halogen C1-5-alkyl; o = 0 - 6 whereby o = 0 when M' is monovalent] followed by reaction with R5CONMeOMe or R5CHO; (e) reaction of II with M''(L')q [M'' = Zn, Cu, Ti; L' = halogen, C1-5-alkyl, PPh3, CN, SCN; q = 0, 1, 2, 3, 4, 5, 6] followed by reaction with R5C(:O)R6, R5C(:O)Me, HC.tplbond.CCR5R6OH or R1CH:CR5R6OH.

IT 853129-78-9 853129-80-3 853129-81-4
853129-82-5 853129-85-8 853129-87-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling reactions of, with aldehydes, amides, ketones and/or epoxides; preparation of vitamin D derivs. starting with monohalovinyl compds.)

RN 853129-78-9 CAPLUS

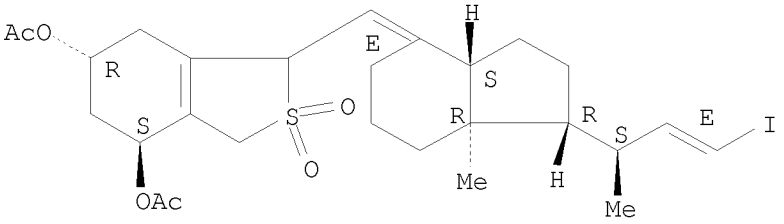
CN Benzo[c]thiophene, 4,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1,3,4,5,6,7-hexahydro-1-[(E)-[(1R,3aS,7aR)-octahydro-1-[(1S,2E)-3-iodo-1-methyl-2-propen-1-yl]-7a-methyl-4H-inden-4-ylidene]methyl]-, 2,2-dioxide, (4S,6R)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



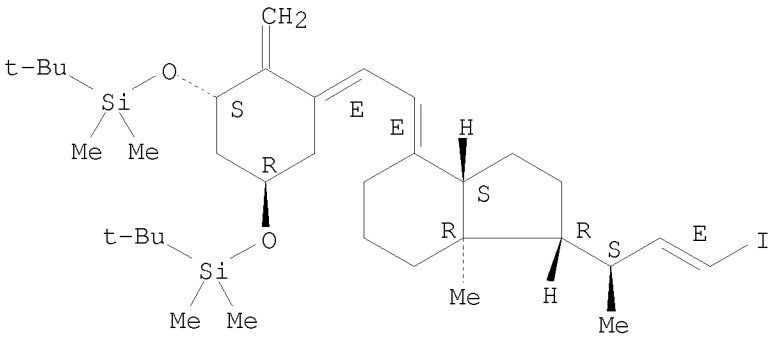
RN 853129-80-3 CAPLUS
CN Benzo[c]thiophene-4,6-diol, 1,3,4,5,6,7-hexahydro-1-[(E)-[(1R,3aS,7aR)-octahydro-1-[(1S,2E)-3-iodo-1-methyl-2-propen-1-yl]-7a-methyl-4H-inden-4-ylidene]methyl]-, 4,6-diacetate, 2,2-dioxide, (4S,6R)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 853129-81-4 CAPLUS
CN 1H-Indene, 4-[(2E)-2-[(3S,5R)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methylenecyclohexylidene]ethylidene]octahydro-1-[(1S,2E)-3-iodo-1-methyl-2-propen-1-yl]-7a-methyl-, (1R,3aS,4E,7aR)- (CA INDEX NAME)

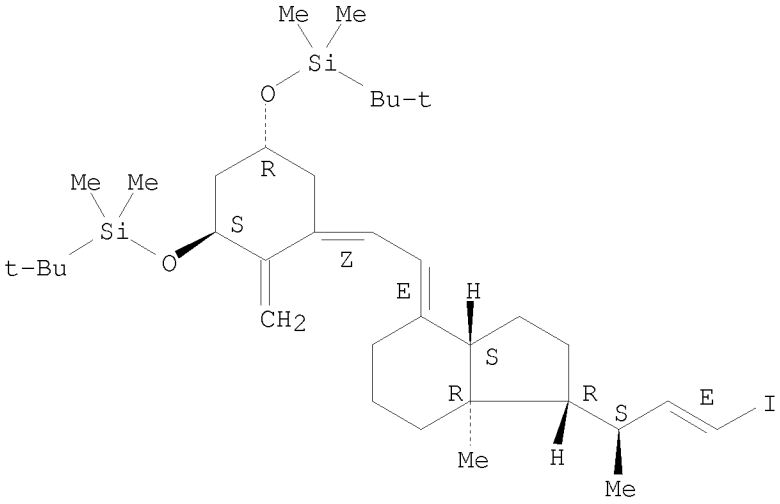
Absolute stereochemistry.
Double bond geometry as shown.



RN 853129-82-5 CAPLUS
CN 1H-Indene, 4-[(2Z)-2-[(3S,5R)-3,5-bis[[(1,1-

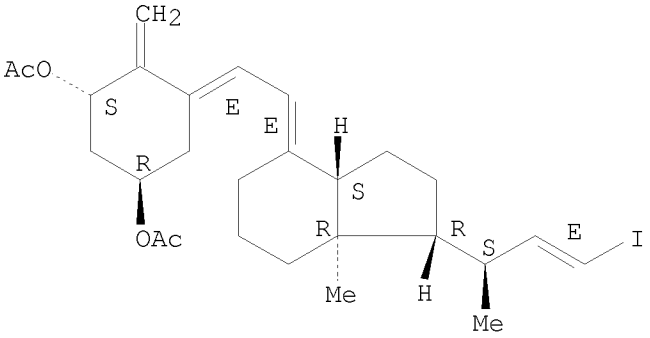
dimethylethyl)dimethylsilyl]oxy]-2-methylenecyclohexylidene]ethylidene]octahydro-1-[(1S,2E)-3-iodo-1-methyl-2-propen-1-yl]-7a-methyl-, (1R,3aS,4E,7aR)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



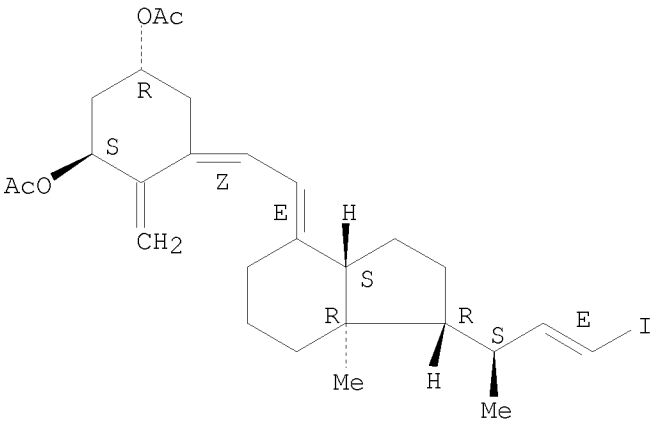
RN 853129-85-8 CAPLUS
CN 1,3-Cyclohexanediol, 4-methylene-5-[(2E)-2-[(1R,3aS,7aR)-octahydro-1-[(1S,2E)-3-iodo-1-methyl-2-propen-1-yl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, 1,3-diacetate, (1R,3S,5E)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 853129-87-0 CAPLUS
CN 1,3-Cyclohexanediol, 4-methylene-5-[(2E)-2-[(1R,3aS,7aR)-octahydro-1-[(1S,2E)-3-iodo-1-methyl-2-propen-1-yl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, 1,3-diacetate, (1R,3S,5Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L5 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:493581 CAPLUS
DOCUMENT NUMBER: 143:26773
TITLE: Process for the preparation of vitamin D monohalogenovinyl derivatives
INVENTOR(S): Buxade Vinas, Antonio; Conchillo Teruel, Antonio; Mola Soler, Carlos
PATENT ASSIGNEE(S): Laboratorios Vinas S. A., Spain
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Spanish
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005051903	A1	20050609	WO 2004-ES511	20041117
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
ES 2233209	A1	20050601	ES 2003-2806	20031128
ES 2233209	B1	20060401		
EP 1688409	A1	20060809	EP 2004-798238	20041117
EP 1688409	B1	20080507		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
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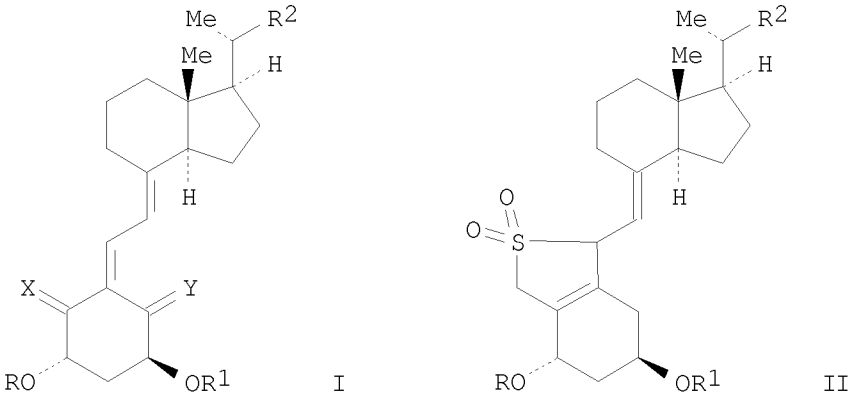
ES 2303111	T3	20080801	ES 2004-798238	20041117

US 20070129558 A1 20070607 US 2006-579594 20060517
PRIORITY APPLN. INFO.: ES 2003-2806 A 20031128
WO 2004-ES511 W 20041117
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 143:26773
GI



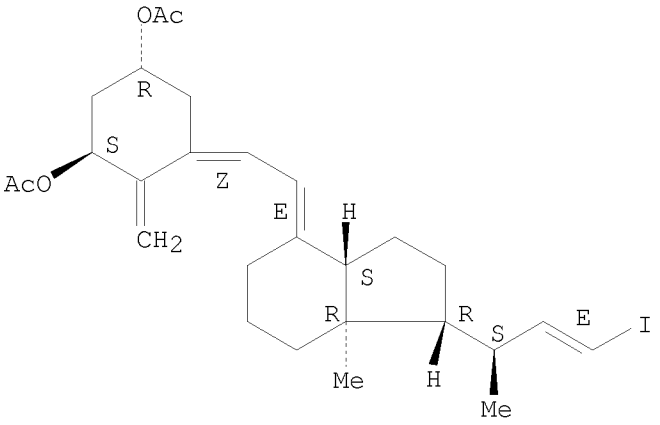
AB A process was disclosed for the preparation of vitamin D 20-(monohalogenovinyl) derivs., such as I and II [R, R1 = H, acyl, silyl, etc.; R2 = CH:CHR3, R3 = halogen; X = CH2, Y = H2; X = H2, Y = CH2], which consisted of reacting an aldehyde precursor I or II (R2 = CHO) with a haloform in the presence of Cr2+ salts. Thus, aldehyde II (R = R1 = SiMe2CMe3, R2 = CHO) was reacted with CHI3 using CrCl2 in THF to give iodovinyl derivative II [R = R1 = SiMe2CMe3, R2 = CH:CHI -(E)] in 80% yield. Iodovinyl derivative II [R = R1 = SiMe2CMe3, R2 = CH:CHI -(E)] was subsequently treated with NaHCO3 in DMF to give I [R = R1 = SiMe2CMe3, R2 = CH:CHI -(E), X = CH2, Y = H2] in 90% yield.

IT 853129-87-0P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(claimed compound; process for the preparation of vitamin D monohalogenovinyl derivs.)

RN 853129-87-0 CAPLUS

CN 1,3-Cyclohexanediol, 4-methylene-5-[(2E)-2-[(1R,3aS,7aR)-octahydro-1-[(1S,2E)-3-iodo-1-methyl-2-propen-1-yl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, 1,3-diacetate, (1R,3S,5Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

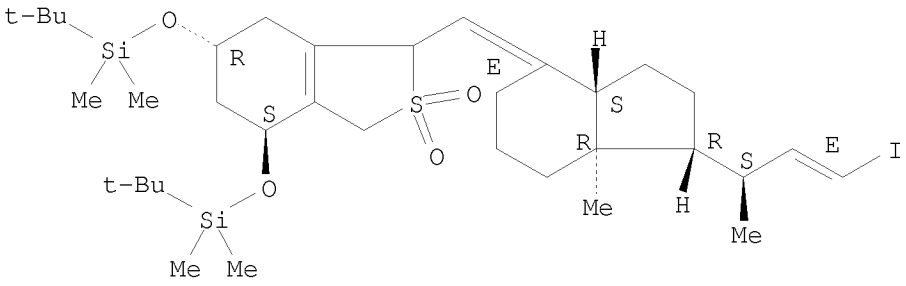


IT 853129-78-9P 853129-81-4P 853129-83-6P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for the preparation of vitamin D monohalogenovinyl derivs.)

RN 853129-78-9 CAPLUS

CN Benzo[c]thiophene, 4,6-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1,3,4,5,6,7-hexahydro-1-[(E)-[(1R,3aS,7aR)-octahydro-1-[(1S,2E)-3-iodo-1-methyl-2-propen-1-yl]-7a-methyl-4H-inden-4-ylidene]methyl]-, 2,2-dioxide, (4S,6R)- (CA INDEX NAME)

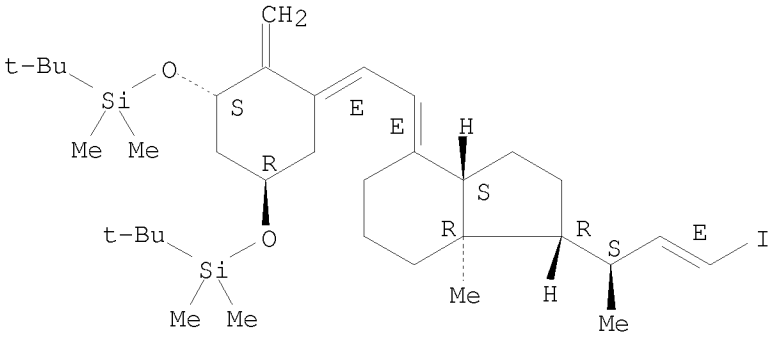
Absolute stereochemistry.
Double bond geometry as shown.



RN 853129-81-4 CAPLUS

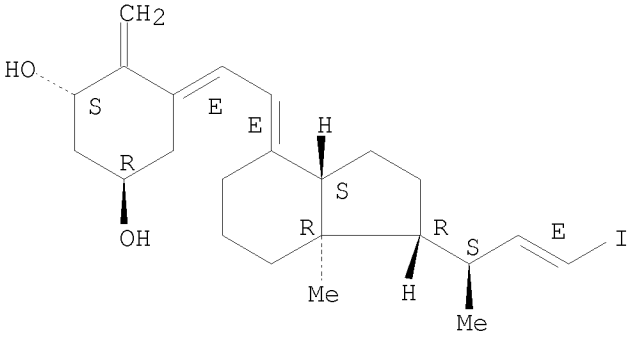
CN 1H-Indene, 4-[(2E)-2-[(3S,5R)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methylenecyclohexylidene]ethylidene]octahydro-1-[(1S,2E)-3-iodo-1-methyl-2-propen-1-yl]-7a-methyl-, (1R,3aS,4E,7aR)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



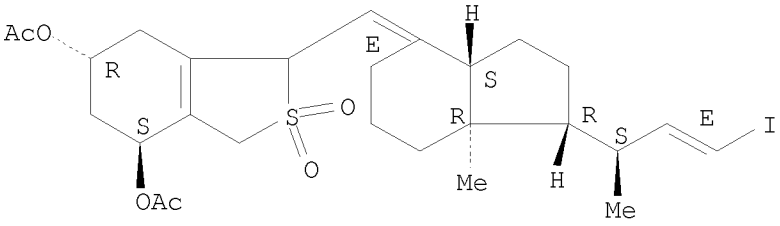
RN 853129-83-6 CAPLUS
CN 1,3-Cyclohexanediol, 4-methylene-5-[(2E)-2-[(1R,3aS,7aR)-octahydro-1-[(1S,2E)-3-iodo-1-methyl-2-propen-1-yl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, (1R,3S,5E)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



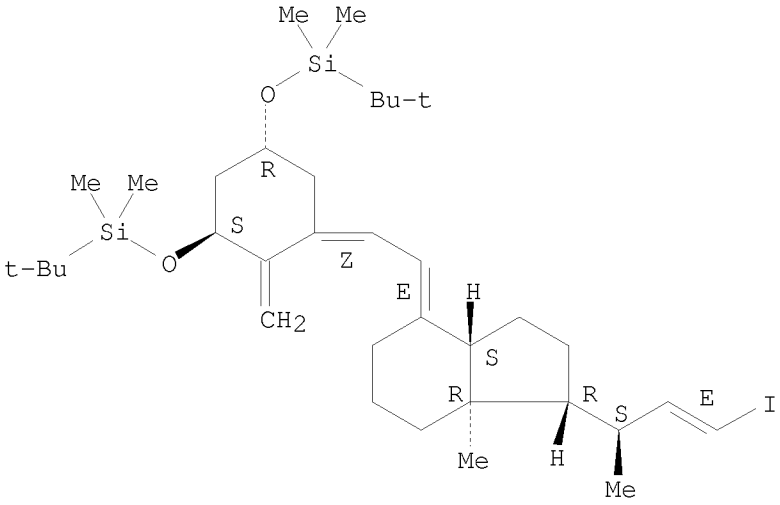
IT 853129-80-3P 853129-82-5P 853129-84-7P
853129-85-8P 853129-86-9P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process for the preparation of vitamin D monohalogenovinyl derivs.)
RN 853129-80-3 CAPLUS
CN Benzo[c]thiophene-4,6-diol, 1,3,4,5,6,7-hexahydro-1-[(E)-[(1R,3aS,7aR)-octahydro-1-[(1S,2E)-3-iodo-1-methyl-2-propen-1-yl]-7a-methyl-4H-inden-4-ylidene]methyl]-, 4,6-diacetate, 2,2-dioxide, (4S,6R)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



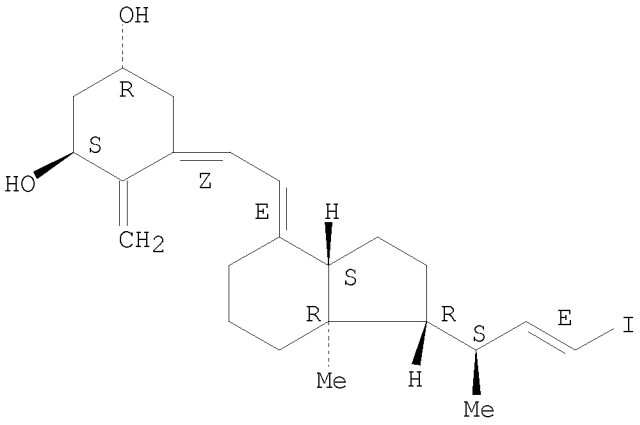
RN 853129-82-5 CAPLUS
CN 1H-Indene, 4-[(2Z)-2-[(3S,5R)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methylenecyclohexylidene]ethylidene]octahydro-1-[(1S,2E)-3-iodo-1-methyl-2-propen-1-yl]-7a-methyl-, (1R,3aS,4E,7aR)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



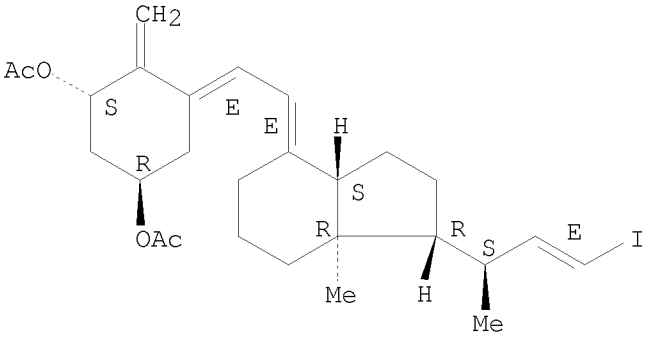
RN 853129-84-7 CAPLUS
CN 1,3-Cyclohexanediol, 4-methylene-5-[(2E)-2-[(1R,3aS,7aR)-octahydro-1-[(1S,2E)-3-iodo-1-methyl-2-propen-1-yl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, (1R,3S,5Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



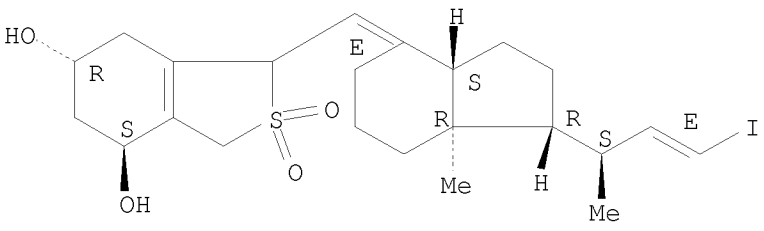
RN 853129-85-8 CAPLUS
CN 1,3-Cyclohexanediol, 4-methylene-5-[(2E)-2-[(1R,3aS,7aR)-octahydro-1-[(1S,2E)-3-iodo-1-methyl-2-propen-1-yl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, 1,3-diacetate, (1R,3S,5E)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



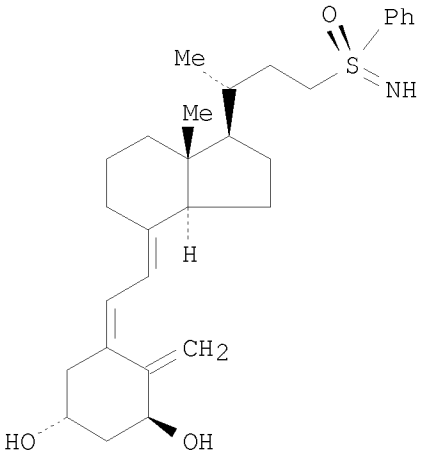
RN 853129-86-9 CAPLUS
CN Benzo[c]thiophene-4,6-diol, 1,3,4,5,6,7-hexahydro-1-[(E)-[(1R,3aS,7aR)-octahydro-1-[(1S,2E)-3-iodo-1-methyl-2-propen-1-yl]-7a-methyl-4H-inden-4-ylidene]methyl]-, 2,2-dioxide, (4S,6R)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as described by E or Z.



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2004:1024083 CAPLUS
DOCUMENT NUMBER: 142:134781
TITLE: Potent, Selective and Low-Calcemic Inhibitors of CYP24 Hydroxylase: 24-Sulfoximine Analogues of the Hormone 1α,25-Dihydroxyvitamin D3
AUTHOR(S): Kahraman, Mehmet; Sinishtaj, Sandra; Dolan, Patrick M.; Kensler, Thomas W.; Peleg, Sara; Saha, Uttam; Chuang, Samuel S.; Bernstein, Galina; Korczak, Bozena; Posner, Gary H.
CORPORATE SOURCE: Department of Chemistry, School of Arts and Sciences, The Johns Hopkins University, Baltimore, MD, 21218, USA
SOURCE: Journal of Medicinal Chemistry (2004), 47(27), 6854-6863
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:134781
GI

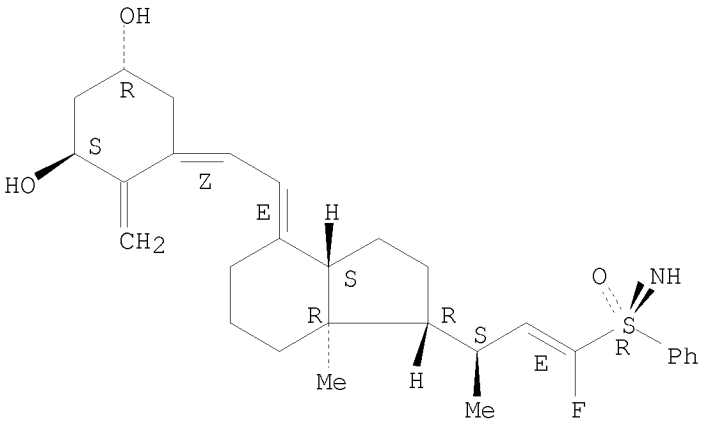


I

AB A dozen 24-sulfoximine analogs of the hormone 1α,25-dihydroxyvitamin D3 were prepared, differing not only at the stereogenic sulfoximine stereocenter but also at the A-ring. Although these sulfoximines were not active transcriptionally and were only very weakly antiproliferative, some of them are powerful hydroxylase enzyme inhibitors. Specifically, 24(S)-NH Ph sulfoximine I is an extremely potent CYP24 inhibitor (IC50 = 7.4 nM) having low calcemic activity. In addition, this compound shows high selectivity toward the CYP24 enzyme in comparison to CYP27A1 (IC50 > 1000 nM) and CYP27B (IC50 = 554 nM).

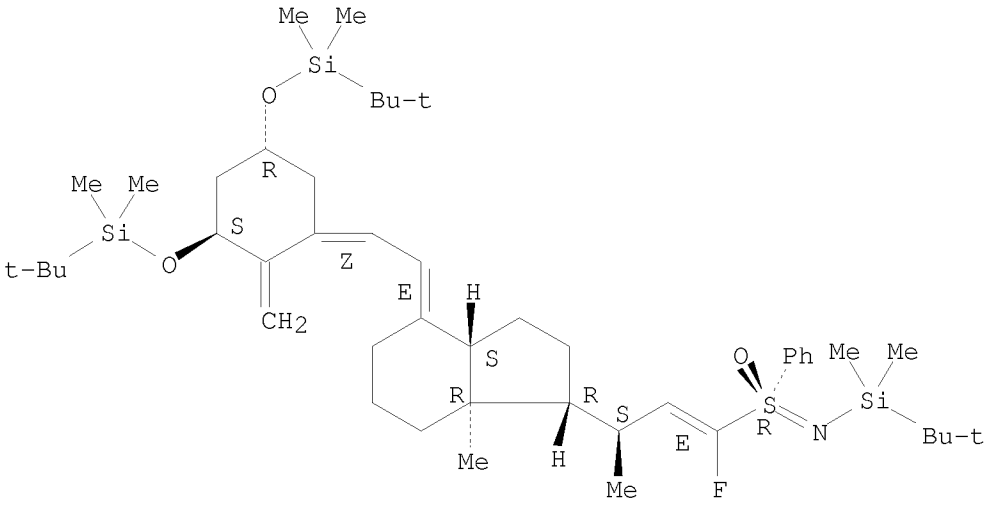
IT 825638-27-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and CYP24 inhibitory activity of dihydroxyvitamin D3 sulfoximine analogs)
RN 825638-27-5 CAPLUS
CN 1,3-Cyclohexanediol, 5-[(2E)-2-[(1R,3aS,7aR)-1-[(1S,2E)-3-fluoro-1-methyl-3-[[S(R)]-S-phenylsulfonimidoyl]-2-propen-1-yl]octahydro-7a-methyl-4H-inden-4-ylidene]ethylidene]-4-methylene-, (1R,3S,5Z)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



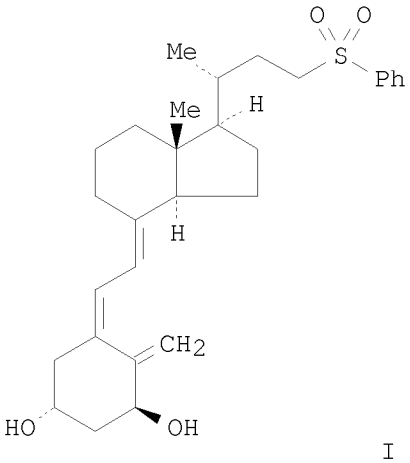
IT 825638-30-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and CYP24 inhibitory activity of dihydroxyvitamin D3 sulfoximine analogs)
RN 825638-30-0 CAPLUS
CN Silanamine, N-[(R)-[(1E,3S)-3-[(1R,3aS,4E,7aR)-4-[(2Z)-2-[(3S,5R)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methylenecyclohexylidene]ethylidene]octahydro-7a-methyl-1H-inden-1-yl]-1-fluoro-1-buten-1-yl]oxidophenyl-λ4-sulfanylidene]-1-(1,1-dimethylethyl)-1,1-dimethyl- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



OS.CITING REF COUNT: 28 THERE ARE 28 CAPLUS RECORDS THAT CITE THIS RECORD (28 CITINGS)
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2004:522160 CAPLUS
DOCUMENT NUMBER: 141:350327
TITLE: Potent, low-calcemic, selective inhibitors of CYP24 hydroxylase: 24-sulfone analogs of the hormone 1α,25-dihydroxyvitamin D3
AUTHOR(S): Posner, Gary H.; Crawford, Kenneth R.; Yang, Hong Woon; Kahraman, Mehmet; Jeon, Heung Bae; Li, Hongbin; Lee, Jae Kyoo; Suh, Byung Chul; Hatcher, Mark A.; Labonte, Tanzina; Usera, Aimee; Dolan, Patrick M.; Kensler, Thomas W.; Peleg, Sara; Jones, Glenville; Zhang, Anqi; Korczak, Bozena; Saha, Uttam; Chuang, Samuel S.
CORPORATE SOURCE: Department of Chemistry, School of Arts and Sciences, The Johns Hopkins University, Baltimore, MD, 21218-2685, USA
SOURCE: Journal of Steroid Biochemistry and Molecular Biology (2004), 89-90(1-5), 5-12
CODEN: JSBBEZ; ISSN: 0960-0760
PUBLISHER: : Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:350327
GI



I

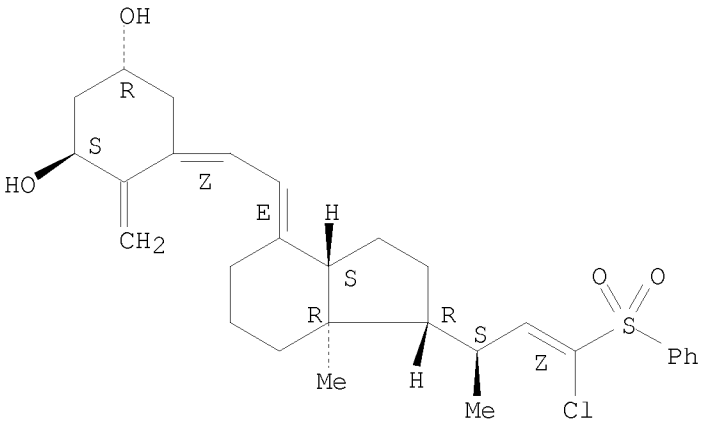
AB The new 24-phenylsulfone I, a low-calcemic analog of the natural hormone 1α,25-dihydroxyvitamin D3, is a potent (IC50 = 28 nM) and highly selective inhibitor of the human 24-hydroxylase enzyme CYP24.

IT 774221-33-9P 774221-34-0P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(24-sulfone analogs of the hormone 1α,25-dihydroxyvitamin D3 as potent, low-calcemic, selective inhibitors of CYP24 hydroxylase)

RN 774221-33-9 CAPLUS

CN 1,3-Cyclohexanediol, 5-[(2E)-2-[(1R,3aS,7aR)-1-[(1S,2Z)-3-chloro-1-methyl-3-(phenylsulfonyl)-2-propen-1-yl]octahydro-7a-methyl-4H-inden-4-ylidene]ethylidene]-4-methylene-, (1R,3S,5Z)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.

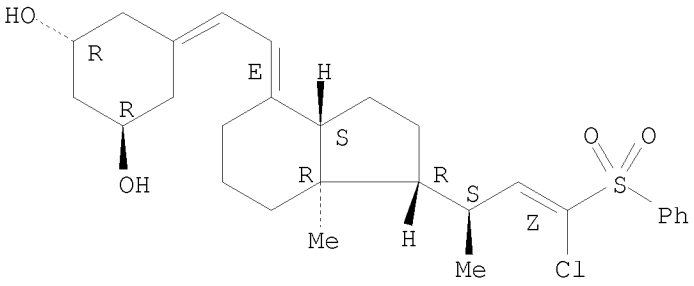


RN 774221-34-0 CAPLUS

CN 1,3-Cyclohexanediol, 5-[(2E)-2-[(1R,3aS,7aR)-1-[(1S,2Z)-3-chloro-1-methyl-3-(phenylsulfonyl)-2-propen-1-yl]octahydro-7a-methyl-4H-inden-4-

ylidene]ethylidene]-, (1R,3R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (19 CITINGS)
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2004:370896 CAPLUS
DOCUMENT NUMBER: 140:391401
TITLE: Preparation of vitamin D analogs as potential phosphate binders, steroids, or anti-proliferative agents
INVENTOR(S): Binderup, Ernst Torndal; Hansen, Kai Holst; Bretting, Claus Aage Svensgaard; Calverley, Martin John
PATENT ASSIGNEE(S): Leo Pharma A/S, Den.
SOURCE: PCT Int. Appl., 68 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004037781	A1	20040506	WO 2003-DK718	20031023
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2500640	A1	20040506	CA 2003-2500640	20031023
AU 2003273781	A1	20040513	AU 2003-273781	20031023
EP 1556345	A1	20050727	EP 2003-757738	20031023
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

BR 2003015553	A	20050823	BR 2003-15553		20031023
CN 1705643	A	20051207	CN 2003-80101931		20031023
JP 2006503880	T	20060202	JP 2004-545731		20031023
RU 2320644	C2	20080327	RU 2005-115482		20031023
MX 2005003499	A	20050617	MX 2005-3499		20050401
IN 2005DN01624	A	20090320	IN 2005-DN1624		20050421
NO 2005002478	A	20050523	NO 2005-2478		20050523
US 20060166949	A1	20060727	US 2005-532019		20051025
PRIORITY APPLN. INFO.:			DK 2002-1608	A	20021023
			US 2002-420783P	P	20021024
			WO 2003-DK718	W	20031023

OTHER SOURCE(S): MARPAT 140:391401
GI

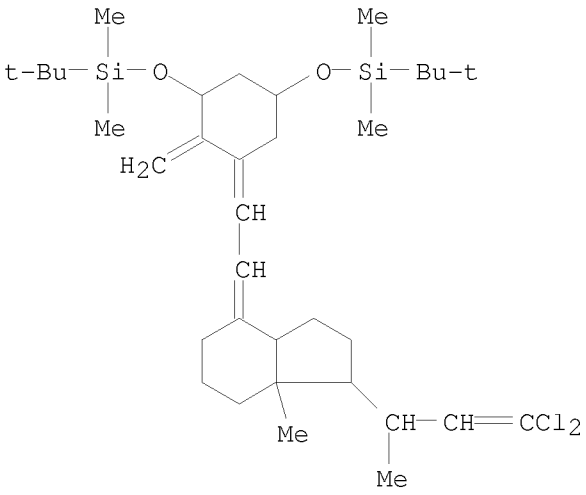
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Vitamin D analogs I (R1 and R2 = halogen, (C1-C6) hydrocarbyl, optionally substituted with one or two hydroxyl group on one or more fluorine atoms, or, together with the carbon atom to which they are both attached, R1 and R2 form a (C3-C6)carbocyclic ring, or one of R1 and R2 taken together with R3 forms a direct bond, such that a triple bond is constituted, or R1 and R2 represent both hydrogen; R3 = a direct bond with one of R1 and R2, hydrogen or (C1-C3)hydrocarbyl; X = (E)-ethylene, (Z)-ethylene, ethynylene, or a bond; Y and Z independently = H or Me; A = OH, F or H; B = CH2 or H2) were prepared as potential phosphate binders, steroids, parathyroid hormone secretion inhibitors, or anti-proliferative agents. Thus, to a solution of II (R = SiMe2CMe3) was reacted with isopropyltriphenylphosphonium iodide to give the corresponding alkene product. The above alkene was treated with anthracene in DCM and irradiated with A TQ718Z2 UV lamp for 35 min to give III (R = SiMe2CMe3) which was treated with tetra-n-butylammonium fluoride trihydrate in THF to give I (A = OH, B = CH2, X = (E)-ethylene, Y = H, Z = Me, R1, R2 = Me, R3 = H).

IT 141545-84-8 154171-12-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of vitamin D analogs as potential phosphate binders, steroids, or anti-proliferative agents)

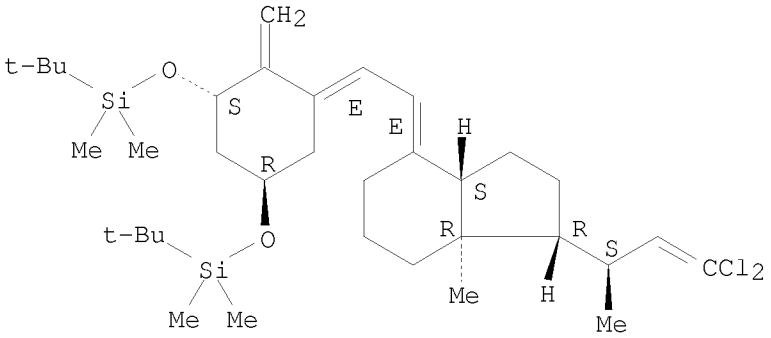
RN 141545-84-8 CAPLUS

CN 1H-Indene, 4-[(2E)-2-[(3S,5R)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methylenecyclohexylidene]ethylidene]-1-[(1R)-3,3-dichloro-1-methyl-2-propen-1-yl]octahydro-7a-methyl-, (1R,3aS,4E,7aR)- (CA INDEX NAME)



RN 154171-12-7 CAPLUS
CN Silane, [[(1α,3β,5E,7E)-23,23-dichloro-24-nor-9,10-secochola-5,7,10(19),22-tetraene-1,3-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl-(9CI) (CA INDEX NAME)

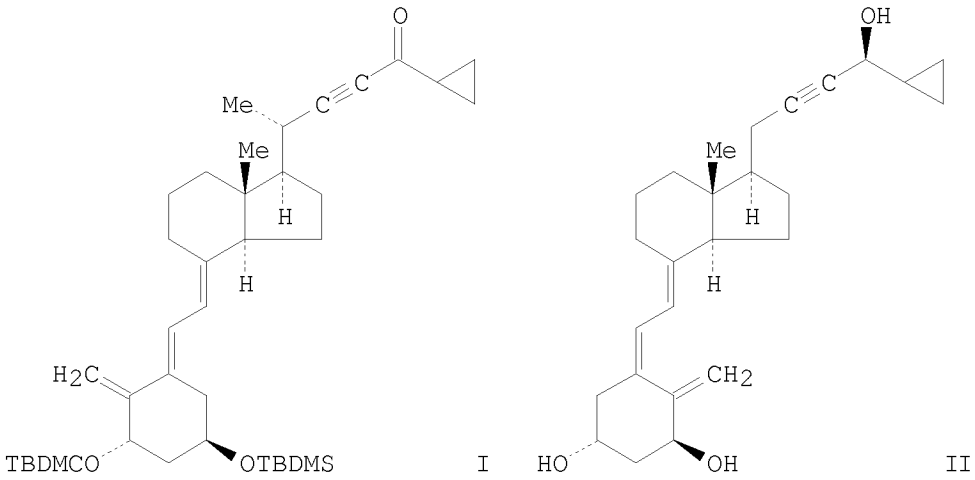
Absolute stereochemistry.
Double bond geometry as shown.



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1994:245588 CAPLUS
DOCUMENT NUMBER: 120:245588
ORIGINAL REFERENCE NO.: 120:43561a,43564a
TITLE: 1α,24S-Dihydroxy-26,27-cyclo-22-yne vitamin D3: the side chain triple bond analog of MC 903 (calcipotriol)
AUTHOR(S): Calverley, Martin J.; Bretting, Claus Aa.S.
CORPORATE SOURCE: Chem. Res. Dep., Leo Pharm. Prod., Ballerup, DK-2750, Den.

SOURCE: Bioorganic & Medicinal Chemistry Letters (1993), 3(9), 1841-4
CODEN: BMCLE8; ISSN: 0960-894X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:245588
GI



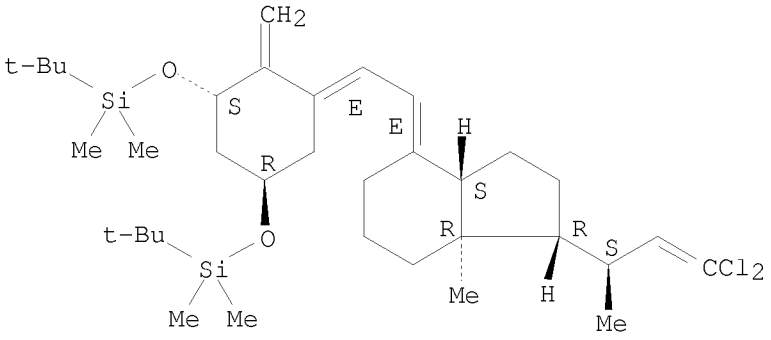
AB The side chain propargylic alc. function [established stereoselectively via S-Alpine-Borane reduction of ynone I (TBDMS = tert-butyldimethylsilyl) and correlated with MC 903] in the title compound II replaces the metabolically labile allylic alc. function of MC 903, a selective analog of the vitamin D hormone used for treating psoriasis. II exhibits reduced in vitro activity but still shows selectively much lower in vivo calcemic effects.

IT 154171-12-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and lithiation and cyclopropylcarbonylation of)

RN 154171-12-7 CAPLUS

CN Silane, [[(1α,3β,5E,7E)-23,23-dichloro-24-nor-9,10-secochola-5,7,10(19),22-tetraene-1,3-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)

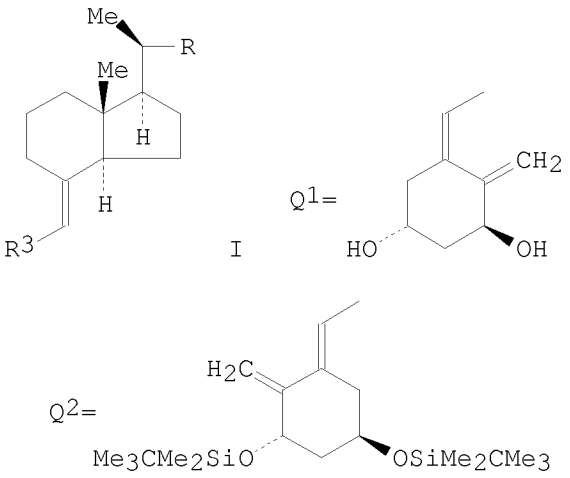
Absolute stereochemistry.
Double bond geometry as shown.



L5 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1992:255875 CAPLUS
DOCUMENT NUMBER: 116:255875
ORIGINAL REFERENCE NO.: 116:43403a,43406a
TITLE: Preparation of vitamin D analogs as drugs
INVENTOR(S): Bretting, Claus Aage Svensgaard
PATENT ASSIGNEE(S): Leo Pharmaceutical Products Ltd. A/S, Den.
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9203414	A1	19920305	WO 1991-DK200		19910711
W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MC, MG, MN, MW, NO, PL, RO, SD, SU, US					
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, ML, MR, NL, SE, SN, TD, TG					
CA 2078555	A1	19920216	CA 1991-2078555		19910711
CA 2078555	C	20021126			
AU 9184223	A	19920317	AU 1991-84223		19910711
AU 636510	B2	19930429			
EP 543864	A1	19930602	EP 1991-914384		19910711
EP 543864	B1	19941214			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE					
JP 06500089	T	19940106	JP 1991-513854		19910711
JP 3246914	B2	20020115			
ES 2068601	T3	19950416	ES 1991-914384		19910711
RU 2126384	C1	19990220	RU 1992-16313		19910711
CZ 286485	B6	20000412	CZ 1992-3726		19910711
US 5447924	A	19950905	US 1992-927420		19920922
FI 103791	B	19990930	FI 1992-5547		19921207
FI 103791	B1	19990930			
SK 281443	B6	20010312	SK 1992-3726		19921217
LV 10089	B	19941020	LV 1993-243		19930215
LT 3666	B	19960125	LT 1993-965		19930910
PRIORITY APPLN. INFO.:			GB 1990-17890	A	19900815
			CS 1992-3726	A	19910711

WO 1991-DK200 A 19910711
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 116:255875
GI

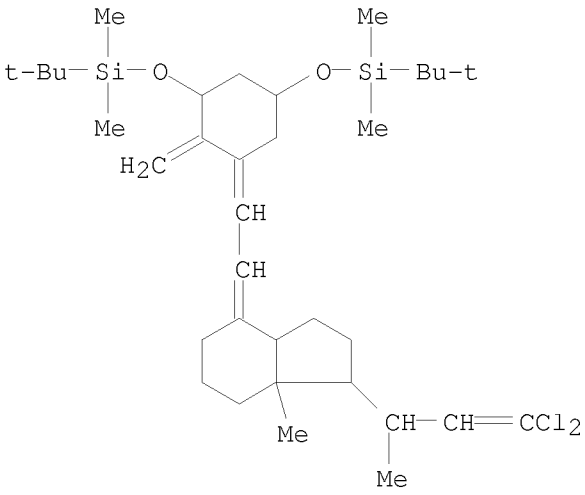


AB Title compds. [I; R = Z1C.tplbond.CZ2CR1R2X; R1, R2 = H, hydrocarbyl; or R1R2 = atoms to form a carbocyclic ring; R3 = cyclohexylidenemethylidyne group Q1; X = H, OH; Z1 = (substituted)(CH2)m; Z2 = bond, hydrocarbylenediyl; m = 0-2] were prepared as antiinflammatories, immunomodulators, etc. (no data). Thus, I (R = CHO, R3 = cyclohexylidenemethylidyne group Q2) was condensed with (Me2N)3P:CCL2 (prepared in situ) and the product treated, in turn, with BuLi and Br(CH2)3CEt2OSiMe3 to give I [R = C.tplbond.C(CH2)3CEt2OSiMe3, R3 = Q2] which was photoisomerized to give, after deprotection, I [R = C.tplbond.C(CH2)3CEt2OH, R3 = Q1].

IT 141545-84-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antiinflammatory and immunomodulator)

RN 141545-84-8 CAPLUS

CN 1H-Indene, 4-[(2E)-2-[(3S,5R)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methylenecyclohexylidene]ethylidene]-1-[(1R)-3,3-dichloro-1-methyl-2-propen-1-yl]octahydro-7a-methyl-, (1R,3aS,4E,7aR)- (CA INDEX NAME)



OS.CITING REF COUNT:	9	THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD (9 CITINGS)
REFERENCE COUNT:	4	THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT